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Error bounds for the integration of singular functions using equidistributed sequences

Elise de Doncker[a,*] and Yuqiang Guan[b]

[a] *Department of Computer Science, Western Michigan University, Kalamazoo, MI 49008, USA*
[b] *Department of Computer Science, University of Texas, Austin, TX 78712, USA*

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Abstract

We consider integral approximations using equidistributed point sequences, which converge for Riemann integrable functions. Under certain conditions, Sobol (Soviet Math. Dokl. 14 (1973) 734) and Klinger (Computing 59 (1997) 223) showed convergence for some classes of singular functions. We focus on asymptotic error bounds and give a scheme for extensions of Sobol's results, thereby obtaining insight in the asymptotic error structure. Numerical examples are presented, validating the principle of "ignoring the singularity" and illustrating the use of extrapolation.

Keywords: Equidistributed point sequence; Singularity; Asymptotic error terms; Extrapolation

1. Introduction

In this paper we consider approximations $Q_N f = \frac{1}{N}\sum_{\rho=1}^{N} f(\vec{x}_\rho)$ to the integral $If = \int_{\mathscr{K}^d} f(\vec{x})\,d\vec{x}$, over the d-dimensional unit hypercube $\mathscr{K}^d$, using equidistributed point sequences $\{\vec{x}_\rho\}$, $\rho = 1, 2, \ldots$. In [5], convergence is shown for a class of singular functions, of the form $f(\vec{x}) = \prod_{i=1}^{d} x_i^{\alpha_i}$, $\alpha_i > -1$, and for certain point sequences. We will be concerned with the leading asymptotic orders in the error, $E_N f = |Q_N f - If|$, of the approximation. In this work we rely on properties of the

*Corresponding author.
E-mail addresses: elise@cs.wmich.edu (E. de Doncker), yguan@cs.utexas.edu (Y. Guan).
URLs: http://www.cs.wmich.edu/˜elise, http://www.cs.utexas.edu/users/yguan.

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integrand combined with discrepancy properties of the point sequences used, to derive a leading asymptotic error sequence.

Whereas we are treating functions which may become singular as soon as any coordinate vanishes, Klinger [1] considers functions of the form $1/(\sum_{i=1}^{d} x_i^{\beta_i})$ with $\sum_{i=1}^{d} \frac{1}{\beta_i} > 1$, and further handles this type of singularity in the interior of $\mathscr{K}^d$. He focuses on the Halton sequence and furthermore on $(0, d)$ point sequences, in order to derive a dominant error bound.

In the next section we will give definitions and review related properties as applicable to one-dimensional problems. Corresponding error bounds are covered in Section 3. Multivariate definitions and notations are given in Section 4. The multi-variate error behavior for a class of functions with boundary singularities of algebraic type is handled in Section 5. Numerical results are reported in Section 6.

2. Basic definitions and properties

Definition 1 (Equidistributed (e.d.) sequence). A (deterministic) sequence $X = \{x_\rho\}_{\rho \geqslant 1}$ is equidistributed (e.d.) or uniformly distributed in $[0, 1]$ if $D_N = o(N)$ as $N \to \infty$, where $D_N = \sup_\ell |S_N(\ell) - N|\ell||$ represents the discrepancy of the sequence $X_N = \{x_1, \ldots, x_N\}$ and $S_N(\ell)$ is the number of points of X_N in the interval $\ell \subseteq [0, 1]$ (of length $|\ell|$).

For later use, we will interpret $S_N(\ell)$, with $\ell = [c, x) \subset [0, 1]$, where $c \leqslant c_N = \min_{1 \leqslant \rho \leqslant N}\{x_\rho\}$ as

$$S_N(\ell) = \sum_{\rho=1}^{N} H(x - x_\rho), \tag{1}$$

with $H(x - x_\rho) = 0$ if $x \leqslant x_\rho$, 1 if $x > x_\rho$.

Theorem 2 (Convergence for Riemann integrable functions). *The point sequence* $X = \{x_\rho\}_{\rho \geqslant 1}$ *is e.d. in* [0,1] *iff* $\lim_{N \to \infty} \frac{1}{N} \sum_{\rho=1}^{N} f(x_\rho) = \int_0^1 f(x)\,dx$ *for every Riemann integrable function* $f(x)$.

As an example, the *Van der Corput sequence* (Sobol's p sequence) [3,5] is defined as follows:

Definition 3 (Van der Corput sequence). $p(\rho) = x_\rho = 0.e_1 \ldots e_m$ if $\rho = e_m \ldots e_1$ (in binary), for $\rho = 1, 2, \ldots$.

3. One-dimensional error

For the class of functions $f(x)$ differentiable for $x>0$ and integrable over $[0,1]$ it can be observed that

Theorem 4 (Convergence). *If* $D_N \int_{c_N}^1 |f'(x)|\,dx = o(N)$ *as* $N \to \infty$, *for the point sequence* $\{x_\rho\}_{\rho \geqslant 1}$ *where* $c_N = \min_{1 \leqslant \rho \leqslant N}\{x_\rho\}$, *then* $\lim_{N\to\infty} \frac{1}{N}\sum_{\rho=1}^N f(x_\rho) = \int_0^1 f(x)\,dx$.

The proof is based on the following equality from [5],

$$\frac{1}{N}\sum_{\rho=1}^N f(x_\rho) - \int_c^1 f(x)\,dx = cf(1) - \frac{1}{N}\int_c^1 (S_N(\ell) - N|\ell|)f'(x)\,dx, \tag{2}$$

with $\ell = [c, x),\ c \leqslant c_N$.

We list this here since a similar approach will be used in the multivariate extension later on. Note that (2) is easy to see using (1) and integration by parts, so that the integral in the right hand side of (2) equals $g(1)f(1) - \int_c^1 g'(x)f(x)\,dx$, where $g(x) = S_N(\ell) - N(x-c)$. Hereby we interpret the derivative of $H(x)$ as the delta function, and also use $g(c)f(c) = 0$ (the latter still holds if $c = c_N = 0$ and $f(c)$ is finite - as for a smooth function).

It then follows from (2) that

$$\begin{aligned}\left|\lim_{N\to\infty} \frac{1}{N}\sum_{\rho=1}^N f(x_\rho) - \int_0^1 f(x)\,dx\right| &\leqslant \lim_{N\to\infty} \frac{1}{N} \sup_{\ell} |S_N(\ell) - N|\ell|| \int_{c_N}^1 |f'(x)|\,dx \\ &\leqslant \lim_{N\to\infty} \frac{1}{N} D_N \int_{c_N}^1 |f'(x)|\,dx = 0.\end{aligned}$$

We can use (2) to bound the error as

$$\begin{aligned}\left|\frac{1}{N}\sum_{\rho=1}^N f(x_\rho) - \int_0^1 f(x)\,dx\right| &\sim \mathcal{O}(c_N) + \mathcal{O}\left(\frac{D_N}{N}\int_{c_N}^1 |f'(x)|\,dx\right) \\ &\quad + \mathcal{O}\left(\left|\int_0^{c_N} f(x)\,dx\right|\right),\end{aligned} \tag{3}$$

as $N \to \infty$.

4. Multivariate definitions and properties

We are now concerned with the error $E_N f = |Q_N f - If|$, of the approximation $Q_N f = \frac{1}{N}\sum_{\rho=1}^N f(\vec{x}_\rho)$ to the integral $If = \int_{\mathscr{K}^d} f(\vec{x})\,d\vec{x}$, over the d-dimensional unit hypercube $\mathscr{K}^d$.

We use the notations from [5] which are listed below.

For $i' = (i_1, i_2, \ldots, i_s)$ where $1 \leqslant i_1 \leqslant i_2 \leqslant \cdots \leqslant i_s \leqslant d$, $1 \leqslant s \leqslant d$, let $P_{i'} = (x_{i_1}, x_{i_2}, \ldots, x_{i_s})$ be a point on the s-dimensional boundary $\mathscr{K}_{i'}$ of the unit cube $\mathscr{K}^d$, on which all the coordinates except for $x_{i_1}, x_{i_2}, \ldots, x_{i_s}$ are equal to 1. Note that $\mathscr{K}_{(1,2,\ldots,d)} = \mathscr{K}^d$.

The region $G_{i'}(c)$ denotes the part of $\mathscr{K}_{i'}$ where the product $x_{i_1} \ldots x_{i_s} \geqslant c$. The s-dimensional rectangular region $\pi_{i'} = \prod_{k=1}^{s} [a_{i_k}, b_{i_k}) \subseteq \mathscr{K}_{i'}$ is of size $|\pi_{i'}| = \prod_{k=1}^{s} (b_{i_k} - a_{i_k})$. Fig. 1 gives illustrations of $G_{i'}(c)$ and $\pi_{i'}$. The point count $S_N^{i'}(\pi_{i'})$ is the number of points in $\{\vec{x}_\rho\}$, $\rho = 1, \ldots, N$, of which the projection $P_{\rho,i'}$ onto $\mathscr{K}_{i'}$ falls into $\pi_{i'}$. The discrepancy (of the projections of the point sequence onto the $\mathscr{K}_{i'}$ boundary) is given by

$$D_N^{i'} = \sup_{\pi_{i'}} |S_N^{i'}(\pi_{i'}) - N|\pi_{i'}||.$$

An equidistributed point sequence in $\mathscr{K}^d$ can be defined analogously with the one-dimensional definition in Section 2 as follows.

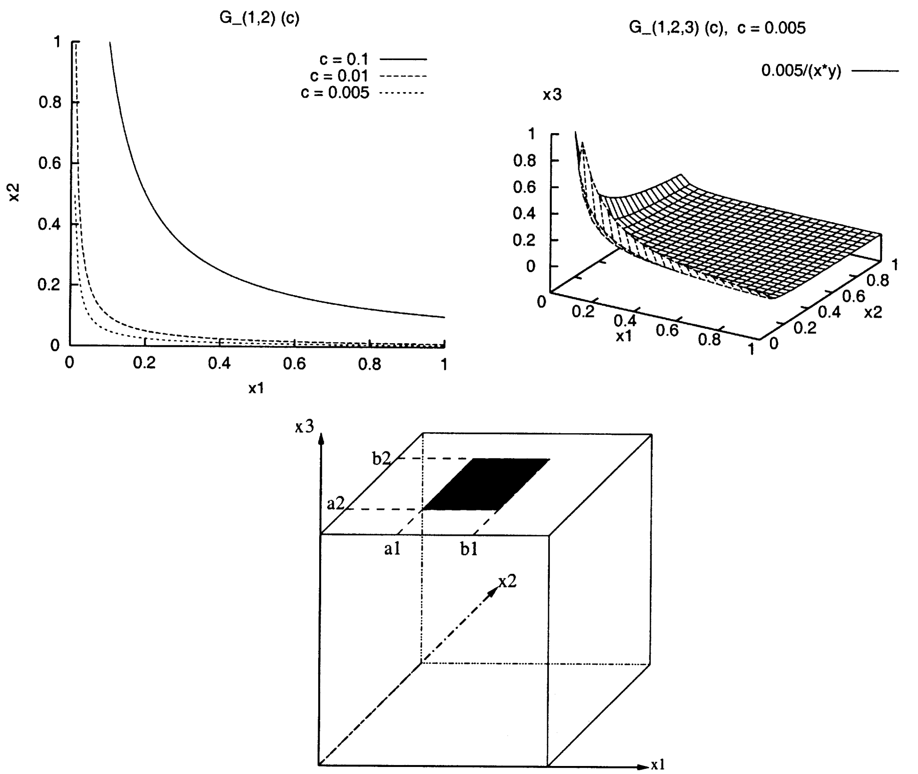

Fig. 1. Illustrations of sample $G_{i'}(c)$ regions (top) and $\pi_{(1,2)} \subset \mathscr{K}_{(1,2)}$ at the boundary of $\mathscr{K}^3$ (bottom).

Definition 5 (E.d. sequence in the unit cube $\mathscr{K}^d$). For an equidistributed sequence $\{\vec{x}_\rho\}_{\rho\geqslant 1}$ in the unit cube $\mathscr{K}^d$, $D_N^{(1,\dots,d)} = o(N)$ as $N\to\infty$.

Theorem 6 (Convergence for Riemann integrable functions). *The point sequence* $\{\vec{x}_\rho\}_{\rho\geqslant 1}$ *is e.d. in the unit cube* $\mathscr{K}^d$, *iff* $\lim_{N\to\infty}\frac{1}{N}\sum_{\rho=1}^N f(\vec{x}_\rho) = \int_{\mathscr{K}^d} f(\vec{x})\,d\vec{x}$ *for every Riemann integrable function* $f(\vec{x})$.

We now focus on a class of integrands $f(\vec{x})$ continuous over $\prod_{\ell=1}^d\ (0,1]$ together with all partial derivatives $f^{(i')}(P_{i'}) = \frac{\partial^s}{\partial x_{i_1}\partial x_{i_2}\dots\partial x_{i_s}} f(P_{i'})$; f may be unbounded as $x_1\dots x_n\to 0$.

Theorem 7 (Convergence). *If* $\int_{\mathscr{K}_{i'}} x_{i_1}\dots x_{i_s}|f^{(i')}(P_{i'})\,dP_{i'}$ *converges for each* i', *and* $D_N^{i'}\int_{G_{i'}(c_N)}|f^{(i')}(P_{i'})|\,dP_{i'} = o(N)$ *as* $N\to\infty$, *for the point sequence* $\{\vec{x}_\rho\}_{\rho\geqslant 1}$ *where* $c_N = \min\{x_{\rho,1}\dots x_{\rho,d}\}$ *for* $\rho = 1,\dots,N$, *then* $\lim_{N\to\infty}\frac{1}{N}\sum_{\rho=1}^N f(\vec{x}_\rho) = \int_{\mathscr{K}^d} f(\vec{x})\,d\vec{x}$.

5. Multivariate error behavior

In order to examine the multivariate error behavior we establish an analogue to (2) by evaluating the s-dimensional integral

$$I(G_{i'}(c))f = \int_{G_{i'}(c)} (S_N^{i'}(\pi_{i'}) - N|\pi_{i'}|)f^{(i')}(P_{i'})\,dP_{i'},$$

where $\pi_{i'} = \prod_{\ell=1}^s\ [c, x_{i_\ell})$, and deriving its relationship with $Q_Nf - If$. In bounding $|Q_Nf - If|$, we use $|I(G_{i'}(c))f|\leqslant D_N^{i'}\int_{G_{i'}(c)}\ |f^{(i')}(P_{i'})|\,dP_{i'}$.

Let us consider the two-dimensional case $f(x_1,x_2) = x_1^\alpha x_2^\beta$. We denote $\vec{x}_\rho = (x_{\rho,1}, x_{\rho,2})$. Similarly to the derivation of (2),

$$\begin{aligned}
I(G_{(1,2)}(c))f &= \int_{G_{(1,2)}(c)} (S_N^{(1,2)}(\pi_{(1,2)}) - N|\pi_{(1,2)}|)\frac{\partial^2 f}{\partial x_{i_1}\partial x_{i_2}}\,dx_1\,dx_2 \\
&= \int_c^1 \int_{\frac{c}{x_2}}^1 \left(\sum_{\rho=1}^N H(x_1 - x_{\rho,1})H(x_2 - x_{\rho,2}) - N(x_1 - c)(x_2 - c)\right) \\
&\quad \times \frac{\partial^2 f}{\partial x_{i_1}\partial x_{i_2}}\,dx_1\,dx_2.
\end{aligned}$$

When $\alpha \neq \beta$, this yields

$$\begin{aligned} I(G_{(1,2)}(c))f = {} & Nf(1,1) - N(1-c)^2 f(1,1) \\ & - \sum_{\rho=1}^{N} f(x_{\rho,1},1) + N(1-c)\int_c^1 f(x_1,1)\,dx_1 \\ & - \sum_{\rho=1}^{N} f(1,x_{\rho,2}) + N(1-c)\int_c^1 f(1,x_2)\,dx_2 \\ & + \sum_{\rho=1}^{N} f(x_{\rho,1},x_{\rho,2}) - N\int_c^1 dx_2 \int_{\frac{c}{x_2}} dx_1 f(x_1,x_2) \\ & + \mathcal{O}(Nc^{\alpha+1}) + \mathcal{O}(Nc^{\beta+1}) + \text{higher order terms}, \end{aligned}$$

which gives

$$\begin{aligned} & \frac{1}{N}\sum_{\rho=1}^{N} f(x_{\rho,1},x_{\rho,2}) - \int_c^1 dx_2 \int_{\frac{c}{x_2}}^1 dx_1 f(x_1,x_2) \\ & \quad = -f(1,1) + (1-c)^2 f(1,1) \\ & \qquad + \frac{1}{N}\sum_{\rho=1}^{N} f(x_{\rho,1},1) - (1-c)\int_c^1 f(x_1,1)\,dx_1 \\ & \qquad + \frac{1}{N}\sum_{\rho=1}^{N} f(1,x_{\rho,2}) - (1-c)\int_c^1 f(1,x_2)\,dx_2 \\ & \qquad + \frac{1}{N}\int_{G_{(1,2)}(c)} (S_N^{(1,2)}(\pi_{(1,2)}) - N|\pi_{(1,2)}|)\frac{\partial^2 f}{\partial x_{i_1}\partial x_{i_2}}\,dx_1\,dx_2 \\ & \qquad + \mathcal{O}(c^{\alpha+1}) + \mathcal{O}(c^{\beta+1}) + \text{higher order terms}. \end{aligned} \tag{4}$$

Note that, when $\alpha = \beta$, terms of $\mathcal{O}(c^{\alpha+1}\log c)$ are introduced.

For $c \sim \frac{1}{N}$, it follows from (4) that

$$\begin{aligned} E_N f \sim {} & \mathcal{O}\left(\frac{D_N^{(1)}}{N^{\alpha+1}}\right) + \mathcal{O}\left(\frac{D_N^{(2)}}{N^{\beta+1}}\right) + \mathcal{O}\left(\frac{D_N^{(1,2)}}{N^{\alpha+1}}\right) + \mathcal{O}\left(\frac{D_N^{(1,2)}}{N^{\beta+1}}\right) \\ & + \mathcal{O}\left(\frac{D_N^{(1)}}{N}\right) + \mathcal{O}\left(\frac{D_N^{(2)}}{N}\right) + \mathcal{O}\left(\frac{D_N^{(1,2)}}{N}\right) \\ & + \mathcal{O}\left(\frac{1}{N^{\alpha+1}}\right) + \mathcal{O}\left(\frac{1}{N^{\beta+1}}\right) + \mathcal{O}\left(\frac{1}{N}\right). \end{aligned} \tag{5}$$

Higher order terms include $\mathcal{O}\left(\frac{1}{N^{\alpha+2}}\right)$, $\mathcal{O}\left(\frac{1}{N^{\beta+2}}\right)$, $\mathcal{O}\left(\frac{1}{N^{2}}\right)$ and $\mathcal{O}\left(\frac{1}{N^{\alpha+\beta+2}}\right)$. When $\alpha = \beta$ or $\beta + 1$, terms of $\mathcal{O}(c^{\beta+2}\log c)$ are also included (terms of $\mathcal{O}(c^{\alpha+2}\log c)$ when $\beta = \alpha + 1$).

A d-dimensional extension, for $f(\vec{x}) = \prod_{i=1}^{d} x_i^{\alpha_i}$, with $-1 < \alpha_i \leqslant 0$ and all α_i distinct, is given by

$$\begin{aligned}\frac{1}{N} I(G_{(1,2,\dots,d)}(c)) f = &\sum_{i' \subseteq (1,2,\dots,d)} (-1)^s \left(\frac{1}{N} \sum_{\rho=1}^{N} f(P_{\rho,i'}) \right. \\ &\left. - (1-c)^{(d-s)} \int_{G_{i'}(c)} f(P_{i'}) dP_{i'} \right) + \sum_{j=1}^{d} \mathcal{O}\left(\frac{1}{N^{\alpha_j+1}} \right) \\ &+ \text{higher order terms.} \end{aligned} \tag{6}$$

Note that, when k of the α_i coincide, terms of $\mathcal{O}(c^{\alpha_i+1} \log^k c)$ are present (as well as, $\mathcal{O}(c^{\alpha_i+1} \log^j c)$, $j = 1, \dots, k-1$).

For $c \sim \frac{1}{N}$, (6) leads to

$$E_N f \sim \sum_{i' \subseteq (1,\dots,d)} \left(\sum_{j=1}^{d} \mathcal{O}\left(\frac{D_N^{i'}}{N^{\alpha_j+1}} \right) + \mathcal{O}\left(\frac{D_N^{i'}}{N} \right) \right) + \sum_{j=1}^{d} \mathcal{O}\left(\frac{1}{N^{\alpha_j+1}} \right) + \mathcal{O}\left(\frac{1}{N} \right).$$

In order to bound $D_N^{i'}$, we first give the following definitions [1–3].

Definition 8 (b-adic interval). A b-adic interval is a subinterval of $[0, 1)$ of the form $[jb^{-v}, (j+1)b^{-v})$ (where j and v are non-negative integers, $0 \leqslant j \leqslant b^v - 1$).

Definition 9 (Elementary box in base b). A product of b-adic intervals in all coordinate directions is an elementary box in base b.

Definition 10 ((τ, d) sequence in base b). For a non-negative integer τ, a point sequence $\{\vec{x}_1, \vec{x}_2, \dots\}$ in $\mathcal{K}^d$ is a (τ, d)-sequence in base b if, for all integers $j \geqslant 0$ and $v \geqslant \tau + 1$, the subset of the points with index ρ such that $jb^v < \rho \leqslant (j+1)b^v$ has the property that each elementary box in base b of size $b^{\tau - v}$ contains b^τ points.

For a (τ, d) sequence with $b = 2$, $D_N^{i'}$ is bounded as follows (see, e.g., [6]):

$$\begin{aligned} &D_N^{i'} = \mathcal{O}(\log^s N); \\ &\text{if } N = 2^v, \quad D_N^{i'} = \mathcal{O}(\log^{s-1} N). \end{aligned} \tag{7}$$

6. Numerical results

For the Van der Corput sequence it can be shown that $c_N \sim \mathcal{O}(\frac{1}{N})$. Furthermore, since it is a $(0, 1)$ sequence, $D_N = \mathcal{O}(\log N)$ and, for $N = 2^v$, $D_N = \mathcal{O}(1)$. For example, letting $f(x) = x^{\beta}$ in (3) gives, as $N \to \infty$,

$$\left| \frac{1}{N} \sum_{\rho=1}^{N} f(x_\rho) - \int_0^1 f(x)\, dx \right| \sim \mathcal{O}\left(\frac{1}{N^{\beta+1}}\right) + \mathcal{O}\left(\frac{\log N}{N^{\beta+1}}\right) + \mathcal{O}\left(\frac{1}{N}\right) + \mathcal{O}\left(\frac{\log N}{N}\right)$$

$$\sim \mathcal{O}\left(\frac{1}{N^{\beta+1}}\right) + \mathcal{O}\left(\frac{1}{N}\right) \quad \text{if } N = 2^{\nu}. \tag{8}$$

As a numerical illustration, after giving the results in tabular form, Fig. 2 (left) graphs results obtained when $\beta = -0.9$, using a sequence of 2^{ν} points, $\nu = 0, 1, \ldots$ (starting with the points $x_1 = 0.5$, $x_2 = 0.25, \ldots$). The graph on the right gives the ratio of the error of the 2^{ν} point result to that of the $2^{\nu+1}$ point result for $\nu = 0, 1, 2, \ldots$. The ratio tends to $2^{\beta+1} = \frac{1}{N^{\beta+1}} / \frac{1}{(2N)^{\beta+1}}$, which corresponds to the dominating error term (for $\beta = -0.9$) in (8).

This leads to the idea of an extrapolation to cancel early terms from the error. Fig. 2 (left) further gives results of a numerical extrapolation assuming an expansion

beta = -0.9
2^(beta+1) = 1.0717734625362931

nu	Result	Error	Ratio	Extrapolated	Error
0	1.8660659830736148	8.133934			
1	2.6741341181290554	7.325866	1.110303	3.4822022531844961	6.518e+00
2	3.2854524043980233	6.714548	1.091044	9.6728392100429836	3.272e-01
3	3.7924136510874398	6.207586	1.081668	10.115045688007378	-1.150e-01
4	4.2359806768869772	5.764019	1.076954	10.009041481895100	-9.041e-03
5	4.6357121046692491	5.364288	1.074517	9.9982800549131543	1.720e-03
6	5.0017585791626988	4.998241	1.073235	10.000036766881120	-3.677e-05
7	5.3398714312896436	4.660129	1.072554	10.000006500958074	-6.501e-06
8	5.6536409623677946	4.346359	1.072191	9.9999998076888268	1.923e-07
9	5.9455501740544054	4.054450	1.071997	9.9999999974609075	2.539e-09
10	6.2174876290601135	3.782512	1.071893	10.000000000105812	-1.058e-10
11	6.4710026577616961	3.528997	1.071838	9.9999999999984102	1.590e-12
12	6.7074347858047281	3.292565	1.071808	9.9999999999998401	1.599e-13
13	6.9279808918953600	3.072019	1.071792		
.	.	.	.		
.	.	.	.		
.	.	.	.		
24	8.5668808553796314	1.433119	1.071773		

Exact: 10.0

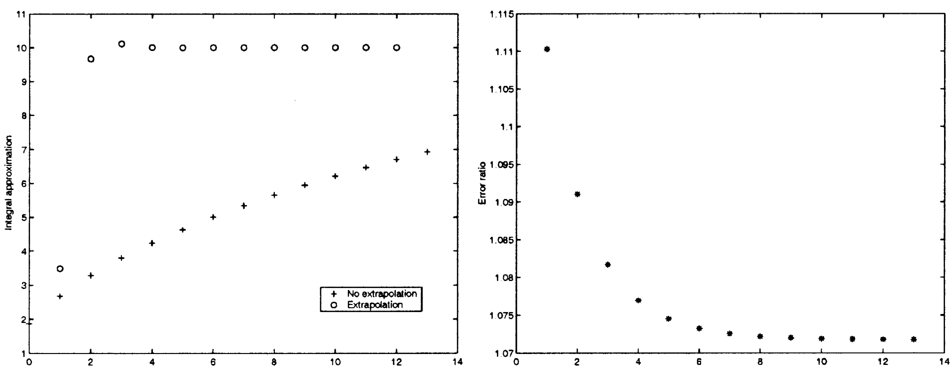

Fig. 2. Integration/extrapolation results and error ratio for $f(x) = x^{-0.9}$.

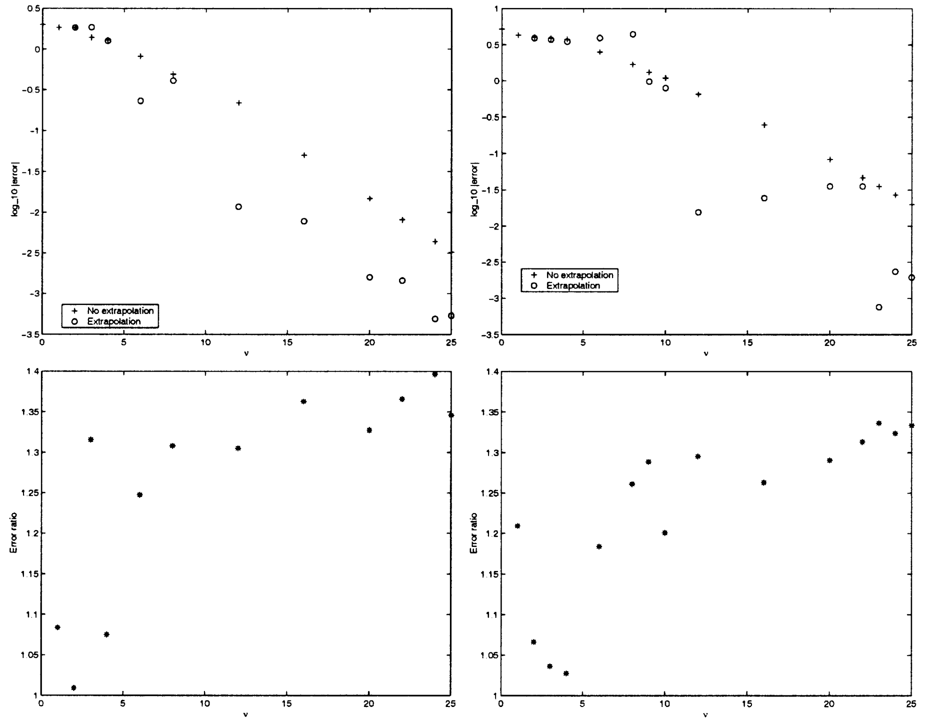

Fig. 3. Integration/extrapolation errors and error ratio for $f(x_1, x_2) = \frac{1}{\sqrt{x_1 x_2}}$ (left) and $f(x_1, x_2, x_3) = \frac{1}{\sqrt{x_1 x_2 x_3}}$ (right) using Sobol point sequences.

of (3) with terms of the form $\mathcal{O}(\frac{1}{N^j})$ and $\mathcal{O}(\frac{1}{N^{\beta+j}})$, $j = 1, 2, \ldots$. The extrapolation was done by solving consecutive linear systems, achieving about 14 digit accuracy at $v = 12$, where the Van der Corput sequence still has an absolute error of 3.29.

Fig. 3 displays results for the functions $f(x_1, x_2) = \frac{1}{\sqrt{x_1 x_2}}$ and $f(x_1, x_2, x_3) = \frac{1}{\sqrt{x_1 x_2 x_3}}$ integrated over $\mathscr{K}^2$ and $\mathscr{K}^3$, respectively. We used the code in [4] to generate the (Sobol) point sequences with 2^v points. The $\log_{10}|\text{error}|$ is displayed on the top; the error ratio on the bottom. Note, for example, that a dominant error term of (exact) order $\mathcal{O}(\log N/\sqrt{N})$ gives a ratio of $\mathcal{O}(\frac{v}{v+1}\sqrt{2})$ (e.g., for $v = 24$ this is $0.96\sqrt{2} \approx 1.36$). The extrapolated sequence is obtained using the ε-algorithm [7] (on the result sequence starting at $v = 0$ and doubling the number of points at each step). The improvements in the extrapolated results appear to occur in stages (corresponding with the elimination of error terms).

For the function $f(x_1, x_2) = \frac{1}{\sqrt{x_1 x_2}}$, the integration results together with the error ratio using the Hammersley (Roth) point sequence $\vec{x}_\rho = (\frac{\rho}{N}, p(\rho))$, $\rho = 1, 2, \ldots$ (which is a $(0, 2)$ sequence) are given in Fig. 4. For example, at $v = 16$, the

nu	Result	Err. ratio	Extrapolated
2	2.100953631303899		
3	2.503843204038287	1.269	
4	2.824031162094882	1.272	4.063672357540369
8	3.575450646443811	1.301	3.988704109752994
12	3.859142813277254	1.326	4.000020357180941
16	3.955965405346892	1.343	4.000000000721994
20	3.986777292136154	1.355	4.000000000138684
21	3.990258414917443	1.357	4.000000000102133
22	3.992834629049205	1.360	4.000000000210599
23	3.994737406187904	1.362	4.000000000079746
24	3.996140243142273	1.363	4.000000000066225
25	3.997172771015135	1.365	4.000000000082220
Exact	4.0		

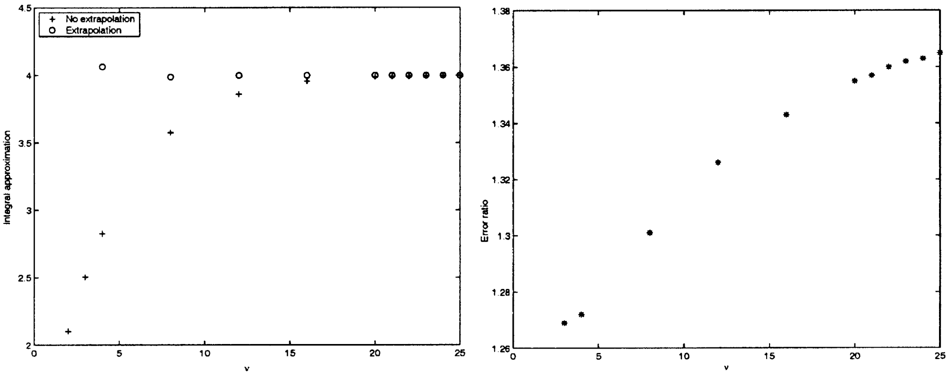

Fig. 4. Integration/extrapolation results and error ratio for $f(x_1, x_2) = \frac{1}{\sqrt{x_1 x_2}}$ using the Hammersley point sequence $\vec{x}_\rho = (\frac{\rho}{N}, p(\rho)),\ \rho = 1, 2, \dots$.

extrapolated result is accurate to about 10 digits, whereas the integration result has about two to three digit accuracy.

The ε-algorithm is known to be effective for extrapolation on sequences with terms of the form $\frac{\log^k N}{N^\alpha}$, k integer $\geqslant 0$, $\alpha > 0$, where N increases as a geometric sequence. As a note of caution, however, it may not work when these are not present in exact order. The process may be slow or unstable when many different types of terms are present.

Further results are given in Fig. 5 (left) for the function $f(x) = \frac{e^x}{\sqrt{x}}$.

For the integration over $[0, 1]$ of a function of the form $f(x) = x^\beta h(x)$, where $-1 < \beta < 0$, and $h(x)$ can be replaced by its Taylor series expansion around $x = 0$, the dominant error behavior is determined by the singular factor.

Some related types of singular functions have been explored. The right part of Fig. 5 shows results for a function with a singularity within the integration interval, $1/\sqrt{|x - \frac{1}{3}|}$. Fig. 6 is for the functions $\log(\frac{1}{x})/\sqrt{x}$ with an algebraic-logarithmic

nu	Result	Error ratio	Extrapolated	Result	Error ratio	Extrapolated
0	0.857763884960707			2.449489742783178		
1	0.701602898861554			1.999341540633072		
2	1.020786514087035	1.67500	0.806461622325341	3.090441045492564	-2.60399	2.318016130217595
3	1.202060914844580	1.62168	1.440336569569936	2.547705216917680	-1.26151	2.727993997305167
4	1.305976670470775	1.55371	1.445544602788551	2.547705216917680	1.02947	2.727993997305167
5	1.368572682830487	1.15005	1.437934458463552	2.610611350364971	1.31644	2.596094794535067
6	1.408322112786291	1.46585	1.508408191968622	2.658958528150115	1.37556	2.614846841274961
7	1.434601583406276	1.44506	1.492915820508541	2.695409910426717	1.39499	2.795898409141889
8	1.452440534559441	1.43290	1.493470223544050	2.721924465319558	1.40315	2.789877628883425
9	1.464746444385010	1.42578	1.493600321408519	2.740957018376996	1.40723	2.788081521940867
10	1.473317027809353	1.42155	1.493634153976432	2.754536929559559	1.40957	2.787796352273945
11	1.479320089032887	1.41897	1.493648837864805	2.764195442564649	1.41103	2.787712025148490
12	1.483539197438047	1.41736	1.493648278361320	2.771051878215636	1.41200	2.787693599317967
13	1.486510747777457	1.41633	1.493648263451000	2.775913231226637	1.41266	2.787693800892475
14	1.488606413752757	1.41565	1.493648264937891	2.779357213400643	1.41312	2.787693737790140
15	1.490085634614484	1.41520	1.493648265593003	2.781795701349016	1.41344	2.787693700282103
		Exact:	1.493648265624853		Exact:	2.787693700234704

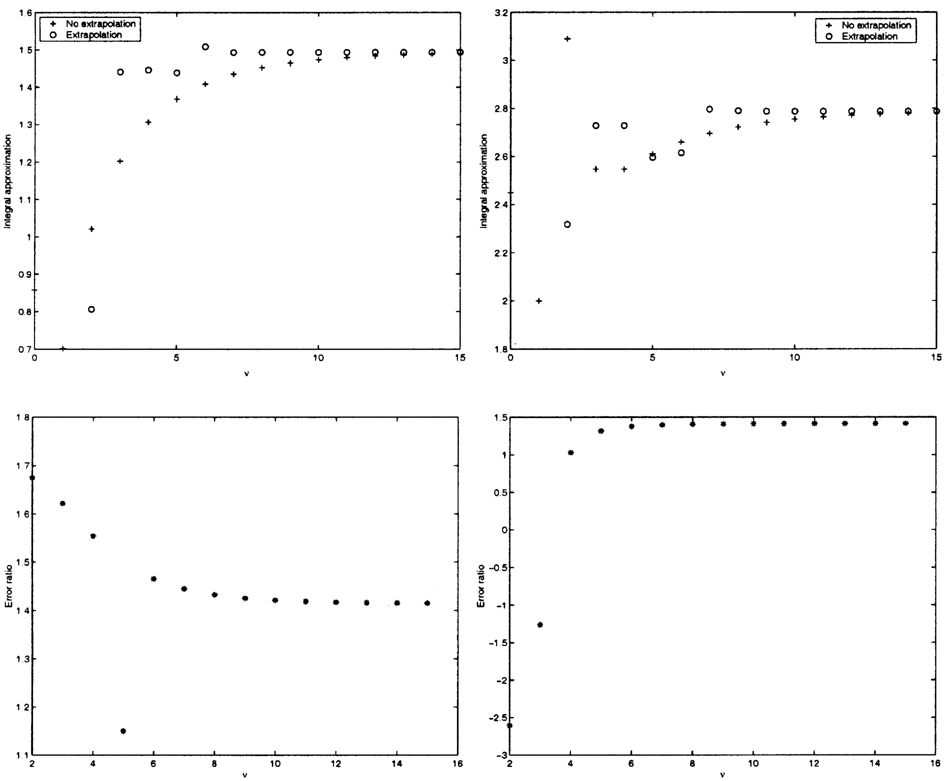

Fig. 5. Integration/extrapolation results and error ratio for $f(x) = \frac{e^x}{\sqrt{x}}$ (left), and $f(x) = \frac{1}{\sqrt{|x - \frac{1}{3}|}}$ (right).

singularity (left), and $x^{-\frac{1}{2}}(1-x)^{-\frac{1}{2}}/(2x+\frac{1}{2})$ with singularities at both endpoints (right). Fast convergence of the extrapolation results is observed.

nu	Result	Error ratio	Extrapolated	Result	Error ratio	Extrapolated
0	0.980258143468547			1.333333333333333		
1	2.021427083228712			1.244016935856292		
2	2.489959540009052	1.29688	0.883883858023514	1.612476960713230	1.30770	1.315906881316421
3	2.853495498116888	1.30312	4.192050950225809	1.991724752671913	1.46351	-11.34086635251196
4	3.133550048171395	1.31028	4.162917439517012	2.265868960418192	1.50389	2.619258684084467
5	3.347889976992517	1.31708	4.228943592611998	2.446658719798649	1.49768	2.758171243858567
6	3.510997886385805	1.32322	3.920207298666138	2.563281398104334	1.47284	2.773562357228959
7	3.634500527656390	1.32869	4.000674099577743	2.639753790084496	1.44938	2.727924787723032
8	3.727606480289967	1.33355	4.000044754549747	2.691219108388483	1.43355	2.811079358952263
9	3.797527059873047	1.33790	3.999999644931754	2.726585630681340	1.42436	2.807668431504559
10	3.849856765308352	1.34181	3.999999993820425	2.751211359804796	1.41941	2.808768130271117
11	3.888901867112573	1.34533	4.000000000026841	2.768485597742211	1.41685	2.809916822067691
12	3.917955130024250	1.34853	3.999999999997733	2.780650599484848	1.41554	2.809925331808786
13	3.939520098341414	1.35145	3.999999999992265	2.789234854440118	1.41488	2.809926005030781
14	3.955490937746430	1.35411	3.999999999996841	2.795298560289563	1.41455	2.809925897396170
15	3.967294631325608	1.35656	4.000000000001219	2.799584024106744	1.41438	2.809925892400491
		Exact:	4.0		Exact:	2.809925892416290

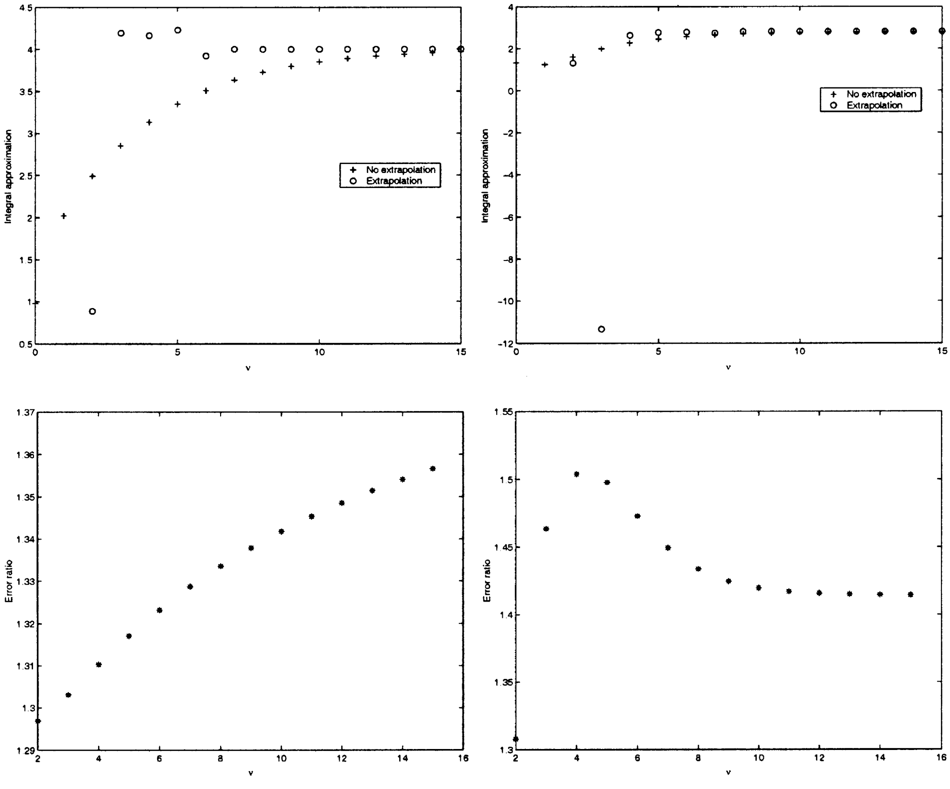

Fig. 6. Integration/extrapolation results and error ratio for $f(x) = \frac{\log(\frac{1}{x})}{\sqrt{x}}$ (left), and $f(x) = \frac{x^{-\frac{1}{2}}(1-x)^{-\frac{1}{2}}}{2x+\frac{1}{2}}$ (right).

7. Conclusions

We obtained asymptotic error bounds and explored the structure of the integration error over the d-dimensional unit hypercube $\mathscr{K}^d$, using equidistributed point sequences, for a class of functions $f(\vec{x})$ (possibly) singular at $x_i = 0$, for $1 \leqslant i \leqslant d$. Our experimental results were in good agreement with the asymptotic error bounds obtained theoretically.

For one-dimensional problems we found that the error expansion warrants extrapolation for functions with algebraic endpoint singularities (using the Van der Corput sequence $\{p(\rho)\}_{\rho \geqslant 1}$). Furthermore, significant convergence acceleration was observed numerically for some logarithmic and interior algebraic singularities.

A multivariate leading asymptotic error expansion was derived for integrands with algebraic singularities at the boundaries of $\mathscr{K}_d$, revealing a complex structure of the error. Extrapolation using the ε-algorithm showed excellent convergence using the two-dimensional Hammersley (or Roth) point sequence $\{(\frac{\rho}{N}, p(\rho))\}_{\rho \geqslant 1}$, where for the number of points N we use successive powers of 2. Examples were given showing convergence acceleration using Sobol point sequences in two and three dimensions. The improvements in the extrapolated results were found to occur in stages. Further research is needed to investigate conditions where exact (tight) orders of the leading error terms can be determined and warrant extrapolation processes.

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